Safeprops: A Software for Fast and Reliable Estimation of Safety and Environmental Properties for Organic Compounds

Jones, Mark Nicholas; Frutiger, Jerome; Abildskov, Jens; Sin, Gürkan

Publication date:
2016

Document Version
Publisher's PDF, also known as Version of record

Safeprops: A Software for Fast and Reliable Estimation of Safety and Environmental Properties for Organic Compounds

Mark Jones[1], Jerome Frutiger[2], Jens Abildskov[2] and Gürkan Sin[2], (1)CAPEC-PROCESS Research Center, Technical University of Denmark (DTU), Lyngby, Denmark, (2)Department of Chemical and Biochemical Engineering, Technical University of Denmark, Kgs. Lyngby, Denmark

We present a new software tool called SAFEPROPS which is able to estimate major safety-related and environmental properties for organic compounds. SAFEPROPS provides accurate, reliable and fast predictions using the Marrero-Gani group contribution (MG-GC) method. It is implemented using Python as the main programming language, while the necessary parameters together with their correlation matrix are obtained from a SQLite database which has been populated using off-line parameter and error estimation routines (Eq. 3-8).

The general form of the MG-GC method is:

$$f_i(X) = \sum N_j C_j + \sum M_k D_k + \sum E_l O_l \quad (1)$$

$$f(X) = T\theta \quad (2)$$

Robust regression is implemented for the parameter estimation. Here the Cauchy weight is used to place high weights on small residuals and small weights on large residuals:

$$\theta^* = \arg\min \sum w_i (y_i^{exp} - y_i^{pred})^2 \quad (3)$$

$$w_i = 1/(1 + (y_i^{exp} - y_i^{pred})^2) \quad (4)$$

Uncertainty of the parameter estimates is based on the asymptotic approximation of the covariance matrix COV(θ*):

$$COV(\theta^*) = SSE/(n - p) * (J(\theta^*)^T J(\theta^*))^{-1} \quad (5)$$

Following the methodology presented by Frutiger et al. [1] [2], the parameter estimates will be described by a student t-distribution:

$$\theta^*_{1-\alpha} = \theta \pm \sqrt{diag(J(\theta^*)COV(\theta^*)J(\theta^*)^T)} * t(n-p, \alpha_t/2) \quad (6)$$

A first guess for the a priori unknown GC factors is provided by applying linear algebra:

$$\theta\hat{} = (T^{tr}T)^{-1} * T^{tr} * f(X) \quad (7)$$

The SAFEPROPS database is accessed to obtain confidence intervals of the property predictions and the following equation is applied:

$$y^{pred}_{1-\alpha} = y^{pred} \pm \sqrt{diag(J(\theta^*)COV(\theta^*)J(\theta^*)^T)} * t(n-p, \alpha_t/2) \quad (8)$$

The software can predict the following safety properties at standard conditions: heat of combustion ($\Delta H_c(T_0)$), the lower and upper flammability limit ($LFL(T_0)$ and $UFL(T_0)$), the auto ignition temperature ($AIT(T_0)$) and the median lethal dose ($LC_{50}(T_0)$). Furthermore, it allows predicting the lower flammability limit at different temperatures (LFL(T)).

The following environmental properties can be estimated: Global Warming Potential (GWP), Ozone Depletion Potential (ODP).

The prediction can be applied to a large variety of chemical compounds including but not limited to hydrocarbons, aromatic compounds, alcohols, acids, esters, ethers, amines, cyclic compounds, hydro-fluorocarbons and chlorine compounds.

The practical application of the software is highlighted in a case study for the screening of organic working fluids for thermodynamic cycles. Safety and environmental constraints should be taken into account as early as possible for the screening of potential working fluid candidates. In this study, a large amount of chemical compounds have been computationally screened. Their performance in the cycle has been analyzed. The corresponding safety-related and environmental properties are then estimated by the new prediction software.

The study shows that the software is a powerful tool for the design of novel organic working fluids, if experimental data is missing.

Finally, a graphical user interface (GUI) is presented which allows the user to search for the compound of interest and obtain the safety and environmental properties including the uncertainty analysis in a tabulated form. An application programming interface (API) is provided to make SAFEPROPS connectible to other modeling environments such as Matlab.

[1] Jérôme Frutiger, Jens Abildskov and Gürkan Sin; A Rigorous Methodology for Development and Uncertainty Analysis of Group Contribution Based Property Models; Abstract from Nineteenth Symposium on Thermophysical Properties, Boulder, United States

[2] Jérôme Frutiger, Camille Marcarie, Jens Abildskov and Gürkan Sin; A Comprehensive Methodology for Development, Parameter Estimation, and Uncertainty Analysis of Group Contribution Based Property Models – An Application to the Heat of Combustion; J. Chem. Eng. Data, 2016, 61 (1), pp 602-613